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A new thermal conductivity model for sandy and peat soils

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ABSTRACT

Soil thermal conductivity (λ) is frequently required when studying coupled heat and water transfer in soils. While λ models are widely available for mineral soil, they are not as readily available for organic soil, which plays an increasingly significant role in climate change and carbon sequestration. This study used a heat-pulse method to measure the thermal properties of six soil peat:mineral mixes spanning wide ranges of water contents and bulk densities. Based on this, a new generalized λ model was proposed, which was tested by fitting the model to heat-pulse measurements, and then comparing with several other widely-used empirical or physically-based models of λ. The new model accounts for the effects of porosity, degree of saturation, organic matter content and soil texture on the thermal conductivity. It is capable of describing the measured data more effectively than other models due to its simplicity and applicability, as indicated by the lowest values of root mean square error (0.028 W m^{-1} K^{-1}) and the highest value of Nash–Sutcliffe efficiency (0.995). The new model has shown potential for use in studying numerical algorithms for describing coupled heat and mass transfer processes in a variety of multiphase soils. It can also be incorporated into global land surface models, particularly in terms of identifying the significance of peat soils on climate change and carbon sequestration.

1. Introduction

Soil thermal conductivity (λ) models are frequently required when studying coupled heat and water transport in the vadose zone, as well as incorporated into global land surface models (Lu et al., 2007). Soil thermal properties are important inputs for models of soil temperature due to the influence of soil temperature on the carbon balance (Kane et al., 1991; Kettridge and Baird, 2007). While the λ of mineral soils have been thoroughly investigated, knowledge of λ for peat soils is limited. Over the past several years the role of peat soils has become increasingly important with respect to climate warming and carbon sequestration, and as a result is receiving increased attention. Consequently, in addition to the accurate measurement of peat soil thermal properties and its controlling factors (Zhao and Si, 2019), it is necessary for the development of appropriate λ models for the high latitude area of peatlands (Kettridge and Baird, 2007).

Theoretically, λ depends on many factors, including the inherent properties such as soil texture and mineral composition (Bristow, 1998; Nikoosokhan et al., 2015) and the porosity-based features such as soil water content (θ) and soil bulk density (ρ) (Abu-Hamdeh and Reeder, 2000). Despite the major progress that is being made in measurement techniques (e.g., heat plate method or heat pulse method) under different influencing factors for various types of soils (Bristow et al., 1994; Campbell et al., 1991), direct measurement of λ remains relatively time consuming, labor intensive, expensive, and impractical for larger-scale applications. Therefore, over the past several decades great efforts have been made to develop λ models which are based on easily measurable soil parameters (Kersten, 1949; De Vries, 1963; Johansen, 1977; Campbell, 1985a,b; Cote and Konrad, 2005; Lu et al., 2007; Pietrak and Wisniewski, 2015).

These λ models may be divided into two general categories: theoretical/mathematical and empirical models (Barry-Macaulay et al., 2015; Dong et al., 2015; Ghanbarian and Daigle, 2016; He et al., 2017). The theoretical/mathematical models assume simplified multi-phase soil systems and heat transfer mechanisms, or have been adapted from predictive algorithms of other properties (e.g., dielectric permittivity). Because the theoretical model is physically based, it requires specific knowledge of soil physical properties and the volumetric fractions of soil components. For instance, de Vries (1963) presented a physically based model which has been widely used with considerable accuracy, but the mineral components and the effects of vapor movement are not easily determined (de Vries, 1958; Horton and Wierenga, 1984;

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Table 1
Properties of soil and peat materials.

	Soil type	Peat:mineral ratio (% g/g)		Particle size distribution			SOC	Soil water content ($cm^3\ cm^{-3}$)	Bulk density ($g\ cm^{-3}$)
	(code)	Peat	Sand	2-0.05 mm	0.05-0.002 mm	< 0.002 mm	(%)		
calibration	Peat-L	100	0	83.7	16.3	0.0	14.48	0, 0.10, 0.25, 0.40, 0.55, 0.70	0.45
	PS23-L	40	60	83.7	16.3	0.0	2.33	0, 0.10, 0.20, 0.30, 0.40, 0.55	1.10
	PS14-L	20	80	83.7	16.3	0.0	1.23	0, 0.10, 0.20, 0.30, 0.40, 0.50	1.30
	Sand-L	0	100	100.0	0.0	0.0	0.29	0, 0.08, 0.16, 0.24, 0.32, 0.45	1.45
	Peat-H	100	0	83.7	16.3	0.0	14.48	0, 0.10, 0.25, 0.40, 0.50, 0.60	0.60
	PS23-H	40	60	83.7	16.3	0.0	2.33	0, 0.10, 0.20, 0.30, 0.40, 0.50	1.30
	PS14-H	20	80	83.7	16.3	0.0	1.23	0, 0.10, 0.20, 0.30, 0.40, 0.45	1.45
	Sand-H	0	100	100.0	0.0	0.0	0.29	0, 0.08, 0.16, 0.24, 0.32, 0.40	1.60
validation	PS41-L	80	20	83.7	16.3	0.0	7.41	0, 0.10, 0.25, 0.40, 0.50, 0.60	0.60
	PS32-L	60	40	83.7	16.3	0.0	4.64	0, 0.10, 0.25, 0.40, 0.50, 0.60	0.90
	PS41-H	80	20	83.7	16.3	0.0	7.41	0, 0.10, 0.25, 0.40, 0.50, 0.55	0.90
	PS32-H	60	40	83.7	16.3	0.0	4.64	0, 0.10, 0.25, 0.40, 0.50, 0.55	1.10

L and H indicate low and high bulk density ranges. SOC is the soil organic carbon content. Peat, PS23, PS14, and Sand samples were used for the model calibration, and PS41 and PS32 samples were sued for the model validation.

Ochsner et al., 2001). The empirical models, on the other hand, are developed based on the analysis of measured λ as a function of combinations of easily available or routinely measured soil parameters, such as θ and ρ. For instance, Kersten (1949) proposed a series of empirical λ equations based on a large number of laboratory measurements. This model only requires ρ as an input parameter, but it is not suitable for predicting λ at relatively low soil water contents. Furthermore, Johansen (1977) proposed a normalized thermal conductivity, i.e., Kersten's number (Ke), and related Ke to the degree of saturation and soil mineral composition. After that, the Johansen (1977) model was improved by effectively reducing the λ estimation errors at relatively low water contents (Cote and Konrad, 2005; Lu et al., 2007). Theoretically, these models may be strongly dependent on the data used for derivation and are not easily applied to other studies or situations. These models also require numerous input parameters, which are not always easily measurable (e.g., quartz content of mineral soils). Thus, there is a need for a λ model that can provide accurate predictions using easily measurable input parameters such as water content and bulk density. One goal of this study was to model the effects of these parameters on the thermal conductivity of a soil in unsaturated and saturated states.

While many studies have investigated the effects of the soil mineral fraction on λ estimations, there are few existing models that consider the influence of soil organic matter content on λ, which is due to the fact that mineral soils normally have low organic matter contents (Balland and Arp, 2005). In permafrost-affected areas, the presence of organic soil (*e.g.*, peat and moss layers) is common (Campbell et al., 2002; Romanovsky and Osterkamp, 2000), and their large amounts of organic matter certainly affect the thermal properties of the soil. In such cases, one solution is to simply apply the theoretical de Vries-based model (1963) to organic soil by considering the organic fraction and its weighting factor. The shape factor for organic matter was previously set as 0.5 (de Vries, 1963); however, the accuracy of this value requires further evaluation using the measured values of λ for organic soils (Tian et al., 2016). Lu et al. (2007) presented thermal conductivity equations for coarse- and fine-textured soils, addressing the importance of the soil textural composition in estimating soil λ values. In addition, few previous studies have evaluated the effects of ρ on λ estimations, which is significant for peat soils because they are easily affected by soil shrinkage. Thus, there is a need to develop a relatively simple, but comprehensive λ function for different θ, soil compositions and ρ values. This function should specifically consider the contributions of organic matter to the soil thermal conductivity.

The current study presents a new generalized model to predict the thermal conductivity of sand and peat soils. In particular, the models between λ of peat soil and its dependent variables were examined under unfrozen conditions; and hence, portions of the analysis and modeling relating to frozen soils (Zhao and Si, 2019) have not been included in this manuscript. The objectives of the study were: 1) to utilize measured data to develop a simple λ model with few parameters that can be easily derived from soil composition and ρ; and 2) to evaluate the suitability and applicability of the new model in predication.

2. Materials and methods

2.1. Treatments

The thermal properties of packed columns (5.5 cm diameter and 11.0 cm height) of 6 constructed soils were measured in a laboratory setting using the heat-pulse method (Li et al., 2016). Both the sand and peat materials used in the soil treatments were taken from the Aurora Soil Capping Study (ASCS) site, Alberta, Canada. Peat soils are organic rich materials with soil organic carbon content about 15%. Peatlands develop in an environment where the annual rate of organic accumulation exceeds the rate of decomposition (Pernitsky et al., 2016). The peat and mineral soils were mixed to different peat:mineral ratios, and particle size distribution and soil organic carbon content were measured (Table 1). The soils were air-dried, ground, and sieved through a 2 mm sieve, and then prepared at various predetermined water contents (volumetric basis). The moist soil was then packed into columns to achieve the desired bulk densities. In total, there were 6 peat:mineral ratios × 2 bulk densities × 5 water contents (Table 1). The bulk density of the different peat-mineral mixes varied between that of pure peat ($0.45\ g\ cm^{-3}$) and pure sand soil ($1.6\ g\ cm^{-3}$), with water contents ranging from relatively dry ($0.08\ cm\ cm^{-3}$) to a saturated ($0.7\ cm\ cm^{-3}$) status, and the soil carbon content ranging between 0 and 14.48%. In addition, the dry state thermal properties were measured after drying the soil sample of the lowest water content completely in an oven for 24 h (70 °C).

2.2. Measurements

The dual-probe heat pulse method was used to measure the soil thermal properties of the prepared soil columns. A dual-probe heat-pulse sensor, consisting of one heater needle and two temperature needles, was vertically inserted from the bottom of each soil column prior to filling it with soil. A CR9000XC datalogger (Campbell Scientific, Logan, UT) was programmed to generate a heat pulse of 60 s and record and store the subsequent temperature change for 1800 s, at

which time it repeated the measurement (Li et al., 2016). The recorded time-series temperature data were analyzed with MathCAD software, following the pulsed infinite line source theory (Bristow et al., 1994). The measurements were repeated seven times, from which the average λ values were calculated.

2.3. Models

Most λ models in the literature are based on empirical relationships or mixing theories. Since there are a limited number of models applicable in peat soils, and the widely used models are somewhat complicated and parameters used are not easy to determine (Farouki, 1981), here we propose a new model of λ. For the purposes of evaluation and comparison, we also examined the widely used 1) a physically-based theoretical de Vries model for thermal conductivity (de Vries, 1963) and 2) an empirical normalized thermal conductivity model (Johansen, 1977; Cote and Konrad, 2005).

2.3.1. Theoretical model (e.g., de Vries model)

The de Vries (1963) model was developed from the Maxwell equation for electrical conductivity of a mixture of granular materials dispersed in a continuous fluid (Eucken, 1932). de Vries (1963) regarded soil as a mixture of ellipsoidal soil particles surrounded by a continuous medium of air or water. Soil λ is estimated with the following equation:

$$\lambda = \frac{f_0\lambda_0 + \sum_{i=1}^{n} k_i f_i \lambda_i}{f_0 + \sum_{i=1}^{n} k_i f_i} \quad (1)$$

where n is the number of ellipsoidal particle types, f_0 and λ_0 are the volume fractions and thermal conductivities (W m^{-1} K^{-1}) of the continuous medium respectively, f_i and λ_i are those values for ellipsoidal particles, and the weighting factor k is given by:

$$k = \frac{1}{3}\sum_{i=1}^{3}\left[1 + \left(\frac{\lambda_i}{\lambda_o} - 1\right)g_i\right]^{-1} \quad (2)$$

where g_i is the shape factor of ellipsoidal particles, and $g_1 + g_2 + g_3 = 1$. For simplicity, assuming g_1 and g_2 are equal, only one shape factor needs to be estimated for each constituent (Li et al., 2016).

For the purposes of this study, we considered our soil samples as a mixture of four constituents (water, air, mineral and organic matter), and we assumed that water was the continuous fluid in all samples. The λ of water, air (vapor), mineral and organic matter is 0.596, 0.025 (0.074), 7.7, and 0.25 W m^{-1} K^{-1} at 20 °C respectively, and the thermal conductivity of the soil solids, λ_s, was chosen for each applicable soil constituent. We considered that the physical properties of soil solid are determined by the soil composition (i.e. the λ_s and g_s are related to the λ and g of mineral and organic matter as follows):

$$\lambda_s = \lambda_m^{f_m}\lambda_o^{f_o} \quad (3)$$

and

$$g_s = g_m f_m + g_o f_o \quad (4)$$

We assumed that $g_m = 0.182$ in terms that our sandy soil is dominated by quartz (Spiers et al., 1989) and $g_o = 0.5$ based on Tarnawski and Wagner (1992).

The shape factor for air follows the assumption of de Vries (1963), varying from a nearly spherical shape ($g_a = 0.333$) in saturated soil to a longitudinal ellipsoidal shape ($g_a = 0$) in nearly dry soil. Following the results of Tian et al. (2016), the g_a was assumed to vary linearly with the soil air fraction (f_a) and was estimated using the following:

$$g_a = 0.333\,(1 - f_a/\eta) \quad (5)$$

where η is the total porosity of the soil. The effects of water vapor on measurements of λ may be significant when using the steady-state method, but this method is unsuitable for the determination of λ in-situ and is rarely used. For the more commonly used heat-pulse method which was applied in the current study, λ can be determined within a short time period of about 2 min, which limits the effects of vapor movement. In addition, all soils were measured at room temperature, and the temperature increases caused by the heat pulse were < 5 °C, indicating that λ of the vapor term is negligibly small (Zhao and Si, 2019).

2.3.2. Empirical model (e.g., Cote and Konrad (2005) model)

There are numerous empirical models that estimate λ. Farouki (1981) reviewed some of the commonly used models for λ, and considered that any of the evaluated models provided acceptable predictions, but the model developed by Johansen (1977) gave the best overall results. Using some of the data provided by Kersten (1949); Johansen (1977) proposed the concept of normalized thermal conductivity, K_e (i.e., the Kersten's number) with respect to the thermal conductivity in dry and saturated states, and established a relationship between λ and K_e for unsaturated soils:

$$\lambda = (\lambda_{sat} - \lambda_{dry})K_e + \lambda_{dry} \quad (6)$$

where λ_{dry} and λ_{sat} are the thermal conductivity of dry and saturated soils, respectively.

Subsequently, this model has been further modified by others, based on their experimental data (e.g., Cote and Konrad, 2005; Lu et al., 2007). In the normalized thermal conductivity model, the determination of K_e is of utmost importance, as the prediction of λ is very sensitivity to the value of K_e. For the Johansen model (1977), K_e is related to the normalized soil water content, but Cote and Konrad (2005) found the model was not accurate when applied at low water contents. Cote and Konrad (2005) adapted the Johansen model (1977) for the prediction of thermal conductivity of pavement base-course materials, and modified K_e to S_r using a soil texture-dependent parameter (m):

$$K_e = \frac{mS_r}{1 + (m-1)S_r} \quad (7)$$

where m = 4.60, 3.55, 1.90, and 0.60 for gravel and coarse sand, medium and fine sand, silty and clay soils, and peat soil, respectively.

Similar to Eq. (3), a geometric mean equation based on the thermal conductivity of water (λ_w) and soil solids (λ_s), was used to estimate λ_{sat}:

$$\lambda_{sat} = \lambda_s^{f_s}\lambda_w^{f_w} \quad (8)$$

where λ_s may be calculated in the same manner as Eq. (3).

The λ_{dry} depends on the soil mineral composition, particle shape, and the volume ratio of air to solids in the soil (de Vries, 1963). Currently, thermal conductivity measurements on dry soils are limited and a general model is in demand to predict λ_{dry} from easily obtainable parameters such as soil texture and porosity. Cote and Konrad (2005) presented a generalized empirical relationship between λ_{dry} and η:

$$\lambda_{dry} = a \times 10^{-b\times\eta} \quad (9)$$

where η is soil porosity, a (W m^{-1} K^{-1}) and b are parameters related to particle shape. a = 1.7, 0.75, and 0.30 and b = 1.8, 1.2, and 0.87 for crushed rocks, sandy soils, and peat soils, respectively.

Eq. (7) is suitable for use with Eq. (6), using lower and upper limit conditions as follows:

lower limit condition: $S_r = 0 \Rightarrow K_e = 0 \Rightarrow \lambda = \lambda_{dry}$

upper limit condition: $S_r = 1 \Rightarrow K_e = 1 \Rightarrow \lambda = \lambda_{sat}$

It is noted that the K_e expressed in either the Johansen (1977) or the Lu et al (2007) models do not satisfy the aforementioned lower limit condition because $\log(S_r = 0) = -\infty$ in the former and $S_r \neq 0$ in the latter. For this reason, the Cote and Konrad (2005) model, i.e., Eq. (7), was the empirical model used in this study for consistent comparison with other types of models.

2.3.3. The new model

Given the wide variety of mathematical expressions used to describe the normalized thermal conductivity for different soil types, a generalized equation valid for all soils would be useful for design engineers and heat flow modelers. Although a certain type of normalized conceptual model (*e.g.*, Cote and Konrad, 2005) performs well in predicting λ for most cases, their model does not always adequately account for the effects of K_e on S_r, especially in fine-textured soils and at lower θ. There are also several models that are not mathematically continuous, and are not physically meaningful of their introduced parameters which may vary greatly depending on the fitted data used for parameter estimation. In contrast, the de Vries model (1963) is widely-used, physically-based, and has been theoretically derived; however, it requires many input parameters (Tarnawski and Wagner, 1992), and the proper selection of parameters, such as critical water content and shape factors (Horton and Wierenga, 1984; Ochsner et al., 2001). In this study, we propose the following logarithmic equation for use across the entire range of soil water contents:

$$\lambda = A + B\ln(1 + S_r) \tag{10}$$

where A and B are soil (composition, texture and structure) dependent parameter, ln is the natural logarithm function, and S_r is the degree of saturation, i.e., ratio between water content and saturated water content which have accounted for the soil bulk density effects.

Note that the equation is continuous, and that A and B may be directly derived from the lower and upper limit conditions as follows:

lower limit condition: $S_r = 0 \Rightarrow \lambda = \lambda_{dry}$ and $\lambda = A \Rightarrow A = \lambda_{dry}$

upper limit condition: $S_r = 1 \Rightarrow \lambda = \lambda_{sat}$ and $\lambda = \lambda_{dry} + B \times \ln(2) \Rightarrow B = (\lambda_{sat} - \lambda_{dry})/\ln(2)$

Given the parameters A and B are actually associated with the thermal conductivity at the two limit conditions, Eq. (10) can be rewritten as:

$$\lambda = \lambda_{dry} + (\lambda_{sat} - \lambda_{dry})\log_2(1 + S_r) \tag{11}$$

If the normalized thermal conductivity concept is used in this equation, then the Kersten's number would be obtained as $K_e = \log_2(1 + S_r)$. From this perspective, the Kersten's number may not depend on soil texture (e.g., Eq. (7)), which can significantly simplify the use of Cote and Konrad (2005) model that are unknown a priori.

In this study, aside from the parameters of the new model (i.e., A and B), which were initially fitted by the measured data, the new model was also evaluated using estimated parameters. For a consistent comparison with two formally discussed models, we used the new model form, but with the λ_{sat} parameters estimated from the Cote and Konrad (2005) model via a two-phase geometric mean model, which is also comparable to the physically-based de Vries model (1963) via a two-phase system method. Similarly, we applied the same model (i.e., Eq. (8)) to calculate λ_{dry}, so as to set up our new model with estimated parameters in a completely physically-based manner.

2.4. Data analysis, model calibration and testing

In processing the data, we were able to represent the graph of the coefficient of thermal conductivity vs the physical properties as a function of the fractional composition of the components of the soil medium, namely the coefficient of water saturation and the peat:mineral ratios. A MathCAD (Prime 2.0, Parametric Technology Corporation) program was developed to find the optimized parameters using the Levenberg–Marquardt algorithm. For the model calibration and validation, the data were separated into two sections (see details in Table 1). The model performance was assessed by plotting the estimated and measured λ associated with 1:1 line, and by calculation of three goodness-of-fit parameters: (1) the root-mean square error (*RMSE*), (2) the average deviations (*AD*), and (3) the Nash–Sutcliff Efficiency (*NSE*):

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2}$$

$$AD = \frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$$

$$NSE = 1 - \frac{\sum_{i=1}^{N}(P_i - O_i)^2}{\sum_{i=1}^{N}(O_i - \bar{O})^2} \tag{12}$$

where N is the number of observations, P_i and O_i are the simulated and measured values, respectively, and $\bar{O}$ is the mean of the observed values. The smaller the *RMSE* is, the higher the model efficiency. The *AD* is equal to zero if the mean and model of the measured values are equal, with over- or under-estimation when above or below zero, respectively. The *NSE* efficiency statistic ranges between 1 and -∞, with 1 indicating a perfect match between observed and modeled values and an *NSE* less than zero indicating that the mean of the observations is a better predictor for $\bar{O}$ than that of the model.

3. Results and discussion

3.1. Thermal properties of sandy and peat soils

The changes in soil thermal conductivity of treatments with varying mineral-organic matter proportions, moisture conditions, and soil bulk densities are presented in Fig. 1. In general, it is clear that λ increased with increased soil water content, sand content, and soil bulk density. The thermal conductivities of the investigated soils ranged from 0.08 W m^{-1} k^{-1} for a dry peat soil to 2.9 W m^{-1} k^{-1} for a saturated sandy soil, with that of the sandy soil is approximately five times greater than that of the peat soil under the same water content and bulk density conditions. With increasing θ, the λ values of course-textured sandy soils sharply increased, while the λ of peat soil increased gradually. Given that air occupies 70% of the total volume in the dry peat soil, the much higher λ_{dry} of the peat soil (0.08 W m^{-1} k^{-1}) than air (0.025 W m^{-1} k^{-1}) could be caused by the existence of preferential heat flow along continuous peat fibers, which contributes to fairly high thermal conductivity (Zhao and Si, 2019). The diverse λ(θ) trends among these soils of different composition can be attributed to the differences in heat conduction in the soil materials themselves, and to the formation of water bridges between soil particles.

For a given bulk density, λ is significantly influenced by θ, as is suggested by the values observed under the nearly saturated condition which are almost twice those for the dry condition. For relatively dry

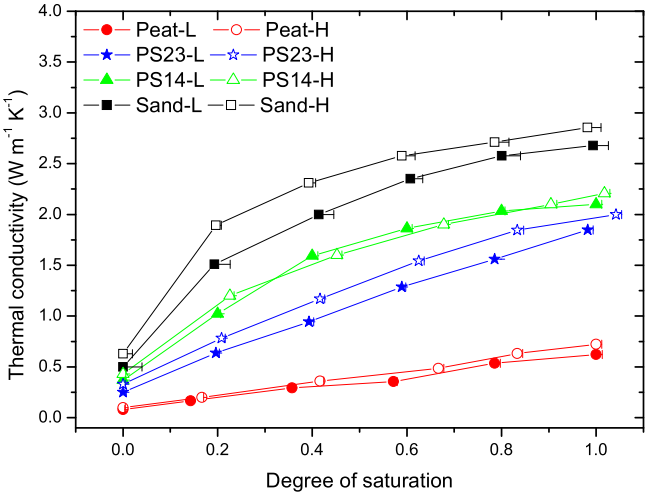

Fig. 1. Soil thermal conductivity (λ) as a function of degree of saturation for four soil types. L and H indicate low and high bulk densities.

soil, water is held tightly on soil particle surfaces by adhesive forces, and the λ remains almost constant because the miniscule amount of water contained in the intra-aggregate pore spaces make an insignificant contribution to heat conduction. As water content increases, soil particles are progressively coated with water, and water bridges are formed between the solid particles. Consequently, an increase in water content increase the area contact between the solid particles and liquid water, displace air, and enhances heat conduction (Ewing and Horton, 2007). Fig. 1 also emphasizes the effects of changing ρ at constant values of θ, indicated that soil λ values decreased by 20% with decreasing ρ.

3.2. General features of the new model

First and foremost, our proposed model has only two unknown parameters, which allows the modelling of soil thermal conductivity as a function of porosity, degree of saturation, and peat/mineral content. Second, the two parameters have strong physical meaning, where A is related to soil porosity and represents the thermal conductivity of soils in dry moisture conditions; and B is related to soil texture and structure, and is associated with the difference between the dry and saturated thermal conductivities. Third, the two unknown parameters may be easily calculated from other easily measured soil properties, which is particularly important when measured λ(θ) data is unavailable for use in fitting the model.

3.2.1. Determination of A

Parameter A is equal to the λ_{dry} in our new model (Eq. (10)). Fig. 2a indicates that the new model with estimated parameters was capable of estimating λ_{dry}. Like the other studies indicated (Cote and Konrad, 2005), estimation of λ_{dry} based on the geometric mean does not fit very well with actual measurement values. However, this approach works as effectively or even better than the other empirical methods, e.g., the Cote and Konrad (2005) model. Therefore, there is still value in using this physically-based approach given that there is no physical meaning associated with the equation parameters for the empirical methods. In general, the thermal conductivity of dry natural mineral soils is correlated to porosity. Cote and Konrad (2005) estimated λ_{dry} ranges from about 0.40 to 0.12 W m^{-1} K^{-1} for porosities ranging from 0.25 to 0.67. In contrast, for a peat soil, λ_{dry} varies from 0.07 to 0.04 W m^{-1} K^{-1} for porosities ranging from 0.72 to 0.96. It is important to note that all methods from the literature which calculate λ_{dry}, are different, are based on their measured data, and do not follow a standardized procedure (Lu et al., 2014). Instead of focusing on the presentation of a function for the calculation of λ_{dry}, we have utilized a two-phase geometric mean model which is the same method used to calculate λ_{sat} or λ_s, handling a universal approach widely used in the literature.

The high ratio of thermal conductivity of solid and air particles (> 100) generally implies a higher sensitivity of the thermal conductivity to the microstructure in dry soils than moist soils (Johansen, 1977). It is difficult to establish the relationship between λ_{dry} and other influencing factors. As indicated by the literature, very few models have been developed to estimate the λ_{dry} value, and the narrow range in soil type and porosity for which they are applicable only offers a reduced possibility of λ_{dry} derivation for the generalized model. Therefore, a physically-based approach has been used in this study to estimate the λ_{dry}. Cote and Konrad (2005) suggested additional improvements be made so that the λ_{dry} model might be applicable to a wider range of soil types, porosities, and degrees of saturation. To date, no theoretical or analytical approaches have been able to quantify the effect of soil mineral composition on λ_{dry} across a wide variety of soil types. The analyses of data from the literature might allow us to develop a generalized physically-based relationship to estimate the λ_{dry} with respect to porosity and the shape of the particles in the soils studied. However, regardless of which form a model uses, physically or theoretically, it is not possible for the suggested λ_{dry} to be a function solely of porosity, it must at least include a dependency on soil texture and/or soil mineralogy. Obviously, it is unreasonable to consider or calibrate λ_{dry} as a function of only porosity (Lu et al., 2014) or bulk density (Johansen, 1977), and it is difficult to define one general form-based, texturally-dependent parameter because the values varied over a wide range (Cote and Konrad, 2005), and the soil mineralogy could be greatly different from one soil to another. Recently, Ghanbarian and Daigle (2016) investigated the soil samples across a series texture used in Lu et al. (2014), and did not find any specific trend between λ_{dry} and soil texture (e.g., clay, silt, or sand content). This again highlights the importance of a physically-based model, like the two-phase geometric mean model utilized in this study.

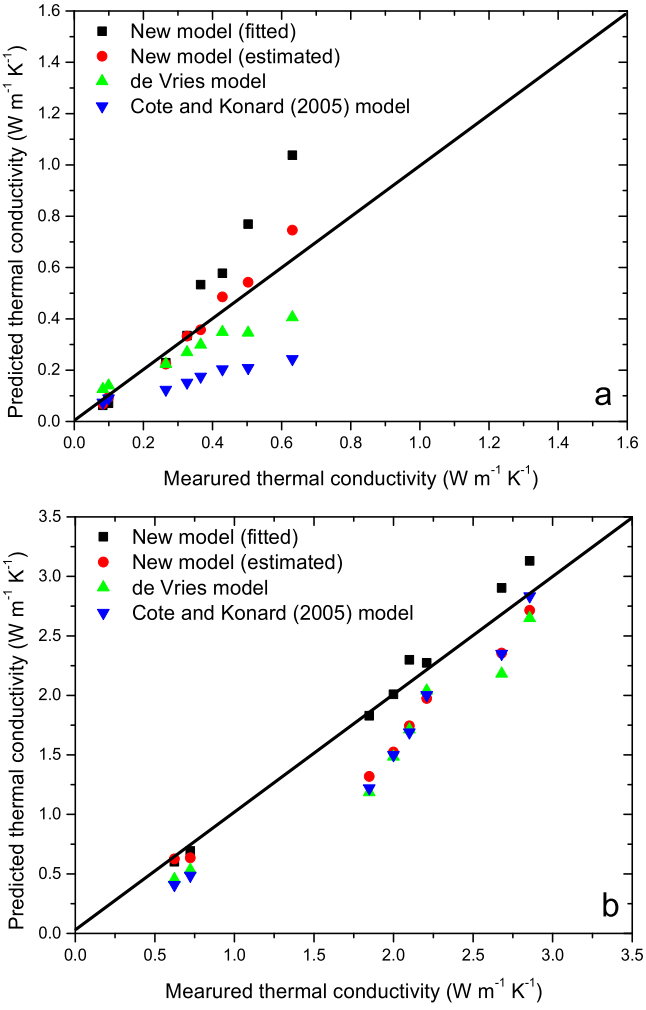

Fig. 2. Comparison of measured and modelled soil thermal properties of four soil types using the new model (fitted and estimated parameters), de Vries model, and Cote and Konrad (2005) model under a) dry condition and b) fully saturated condition.

3.2.2. Determination of B

Parameter B is equal to (λ_{sat} - λ_{dry})/ln(2) in our new model. Two-phase saturated systems have been widely employed to predict λ_{sat} (Progelhof et al., 1976), with the geometric mean model proposed by Woodside and Messmer (1961) being the most frequently used. Fig. 2b shows that the new model with estimated parameters underestimates λ_{sat}, similar to the underestimation of λ_{dry}. However, the new model with estimated parameters is comparable to the Cote and Konrad (2005) and de Vries (1963) models. The new model and Cote and Konrad (2005) model retained the same calculation of λ_{sat}, and the physically-based version of de Vries model is also very similar to these

models. This provides confirmation that the current physically-based geometric mean approach is quite reliable for predicting λ_{sat}.

Our results imply that, without any thermal conductivity measurement data, the new model could provide similar predictions of λ in the wet range than that in the dry range. This is inconsistent with other studies (Lu et al., 2014; Tian et al., 2016), which generally considered that the geometric mean approach is only applicable to the prediction of λ_{sat}. The quantity of measurement data for λ_{sat} or λ_{dry} within the literature is very limited and presents difficulties when attempting to evaluate the accuracy of the associated models. Evaluations using data from the literature (Lu et al., 2007), and in-situ soil measurements, showed that the predicted values of thermal conductivity from the proposed model agreed well with the measured data, for a wide range of soil textures. On the in-situ clay loam soil, the less important dry bulk density effect on the thermal conductivity at dry state (λ_{dry}) was confirmed. It has also been observed that the λ_{sat} is partially dependent on both the content of sand and the dry bulk density. Kersten's (1949) research, which still remains the only comprehensive study of its kind, provided sufficient information on the materials studied in the estimation of the λ_{dry} and λ_{sat} values for various soils. From our perspective, it is more important to determine specific λ_{dry} and λ_{sat} values, especially λ_{dry}, and to establish physically-based models and parameters using those values, than it is to suggest and evaluate the form of λ.

In comparison the estimation of λ_{sat} and λ_{dry} between soil types, while the accuracy of prediction of λ_{sat} is very similar for different soil types, but the errors in predicting λ_{dry} are larger for the sandy soil than for the peat soil (Fig. 2a). This suggests that the method we provided for the estimation of λ_{dry} is very effective, especially for the peat soil in the permafrost region.

3.3. Model valuation and comparisons

As shown in Fig. 3, the new model based on fitted parameters performs better than the Cote and Konrad (2005) model and de Vries model in predicting the λ(θ) relationship for all tested soils, providing the lowest *RMSE* (0.028–0.228) and the largest *NSE* (0.825–0.995) (Table 2). The Cote and Konrad (2005) model and de Vries model underestimated λ(θ) across the full textural range of soils, especially for those under near-saturated conditions. This underestimation occurs primarily because the estimated values of λ_{sat} are smaller than the measured ones, and because the measurement errors are not evenly distributed over the entire range of θ. Similarly, the new model using estimated parameters, in which both λ_{sat} and λ_{dry} are based on the geometric mean equation, underestimated λ(θ) over the full textural range of soils. Interestingly, the predictions generated from the new model when using an estimated parameter value, were very comparable to the results obtained with the Cote and Konrad (2005) model and de Vries model.

Furthermore, the curves of λ(θ) based on the estimated parameters are lower but parallel to those based on the fitted parameters (Fig. 3). This trend indicates that the parameter values are important factor in predicting the thermal conductivity. In addition to the underestimation of λ_{sat}, it shows that the method which uses the geometric mean equation underestimates λ_{dry} as well. These larger observed λ(θ) values could be also the result of a bias caused by vapor transport, given that it was not well considered in the estimation. Farouki (1981) indicated that the major errors associated with the de Vries model arise from the assumption that soil particles are not in strong contact with each other (*i.e.*, weak continuous medium for air), and a 25% increase is suggested to the original λ estimation for dry soils. The approximation procedure outlined by de Vries (1963) for estimating particle shape factors also produces errors in λ estimations. For comparison of different soil textures, the Cote and Konrad (2005) model and de Vries model perform better for fine- to medium-textured soils than for the coarse-textured ones (sands). These results agree with those of Barry-Macaulay et al. (2015) who found these models gave unsatisfactory λ(θ) values in sands of lower water contents. Dong et al. (2015) assessed the performance of the Cote and Konrad (2005) model using three soils, and found that the model showed a similarly increasing trend with the experimental data, but the model did not satisfactorily estimate the λ(θ) values for sands at saturation. Cote and Konrad (2005) and Lu et al. (2007) recommended different parameter values for different soil textures, but no quantitative thresholds were provided to distinguish the boundaries between textures. For example, Cote and Konrad (2005) use soil texture-dependent parameters of 4.60 and 1.90 for gravel and coarse sand, and silty and clayed soils, respectively, while Lu et al. (2007) suggested 0.96 and 0.27 for coarse- and fine-textured soils, respectively. Different parameter values may result in a different K_e for the same soil, which indicates there are challenges associated with defining the parameter(s) due to the lack of a solid theoretical concept. Such parameters, therefore, need to be determined by directly fitting those models to experimental measurements or by inversion of a numerical simulation model. Therefore, in addition to the best fitted parameter for the newly developed model, evaluating the model using previously estimated parameter(s) is also important. For example, relating the soil-type factor in Cote and Konrad (2005) model to other soil parameters requires minimal knowledge of geotechnical properties, but can be extremely useful for comparative purposes. The particle size distribution would be a good indicator for characterizing different soil types; however, the only available data are partial distributions provided by Kersten (1949), so parameter values cannot be precisely determined in this manner. Additionally, due to its highly fibrous texture, the diameters of peat solid particles cannot be characterized in the same manner as those of conventional mineral soils (gravel, sand, silt, and clay). However, it is known that grain-size distribution, together with the shape of the particles, will affect the packing geometry and soil bulk density. For example, gravel with widely distributed particle sizes can be prepared with lower porosities (higher bulk densities) than fine sand with a uniform particle size. This indicated that the bulk density, which has been taken into account in our new model, could be better utilized in parameter estimation of thermal conductivity models.

It is important to note that the development of the Johansen (1977) and Cote and Konrad (2005) models relied on measured data sets, whereas the development of the new model was based on a physical equation and is independent of measured data sets. Commonsensically, empirical models agree well with the soil property used in the model derivation and calibration, but the model may not be well adapted for use with other soils that have a different range of properties. This dilemma also presents itself in the Johansen (1977) model, which was found to be sensitive to quartz content and soil porosity, and prone to errors in estimating λ at lower water contents (Cote and Konrad, 2005). Many efforts have been made to improve the Johansen (1977) model (Cote and Konrad, 2005; Lu et al., 2007, 2014), but very few models are applicable for a variety of soil types and water contents.

Recently, Ghanbarian and Daigle (2016) developed a theoretical model (GD model) for thermal conductivity via the percolation-based effective-medium approximation. Compared with our model, it employed mathematical derivation processes, although it has similar model parameters with our model. Given the very limited theoretical model available, it is valuable to test this model using our data. What is more, it has not been evaluated for use with organic soils. Since all soil peat:mineral mixes have zero clay content (Table 1), we accordingly calculate critical water content is 0 and scaling exponent (t_s) is 0.342 in such soil packs. Using the available and measured porosity, λ_{dry}, and λ_{sat} values, we then estimated the saturation-dependent thermal conductivity via the GD model ($\lambda = (\theta_s - \theta)/\theta_s * \lambda_{dry}^{1/t_s} + \theta/\theta_s * \lambda_{sat}^{1/t_s})^{t_s}$; Sadeghi et al. (2018)). Except for the different forms of those two models, the method used to calculate λ_{dry} is different. While the geometric mean equation was applied to estimate the λ_{dry} in our model, GD model estimated the λ_{dry} via the suggested empirical equations from Cote and Konrad (2005), i.e., Eq. (9) in this study. Fig. 4 showed a

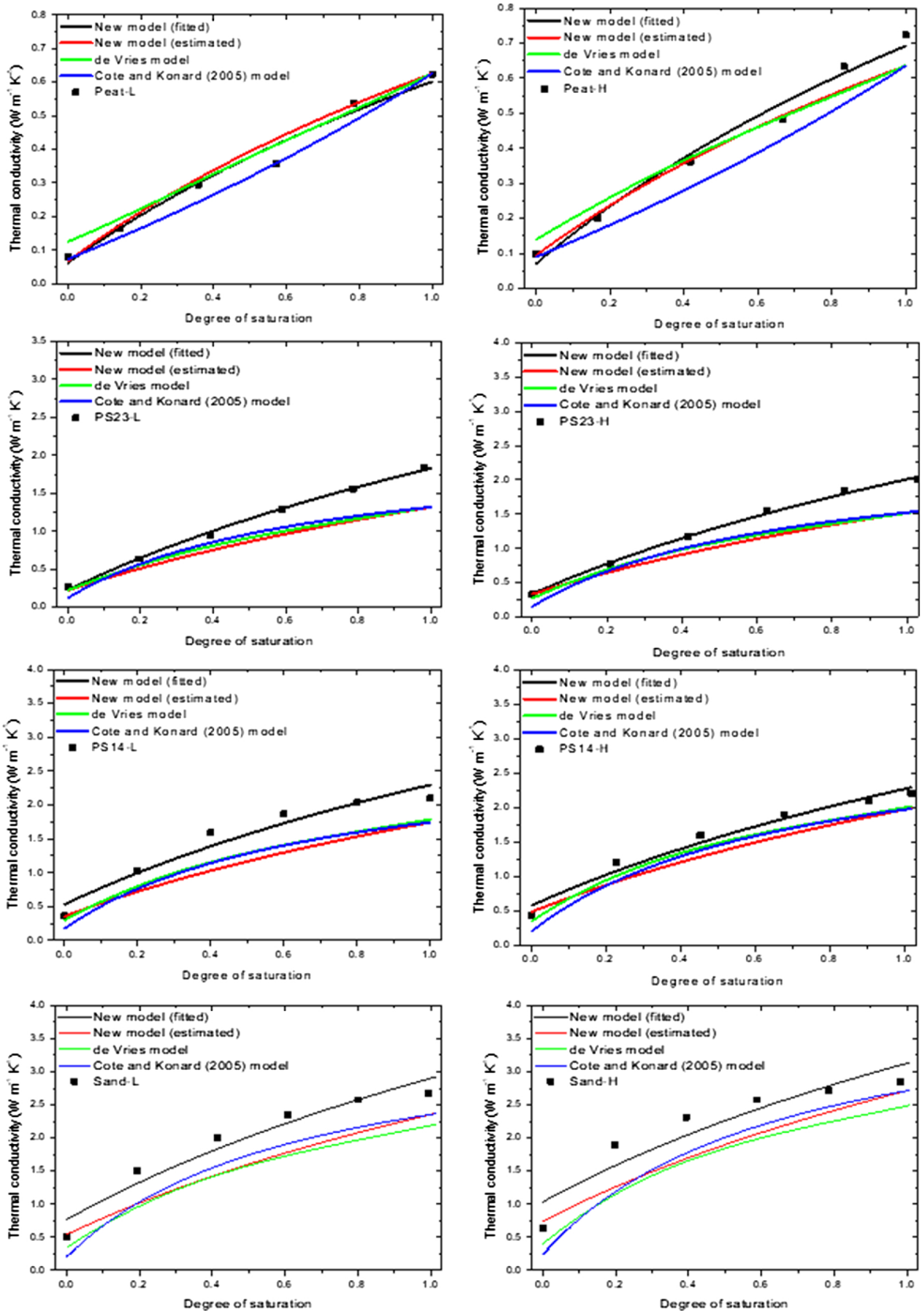

Fig. 3. A comparison of measured and modeled soil thermal conductivity-water content relationships for four soil types, including the new model (fitted and estimated parameters), de Vries model, and Cote and Konrad (2005) model. L and H indicate low and high bulk densities.

Table 2
Model performance of tested samples based on *RMSE*, *AD* and *NSE* with the new model (fitted and estimated parameters), de Vries model, and Cote and Konrad (2005) model for four soil types.

Soil type	*RMSE*				*AD*				*NSE*			
(code)	Fitted	Esti -mated	deVries	Cote and Konrad	Fitted	Esti -mated	de Vries	Cote and Konrad	Fitted	Esti -mated	de Vries	Cote and Konrad
Peat-L	0.029	0.035	0.030	0.035	0.004	0.021	0.016	−0.025	0.964	0.953	0.962	0.961
PS23-L	0.029	0.357	0.335	0.314	0.007	−0.324	−0.290	−0.260	0.995	0.309	0.279	0.284
PS14-L	0.141	0.470	0.383	0.401	−0.034	−0.457	−0.372	−0.394	0.907	0.349	0.431	0.417
Sand-L	0.161	0.500	0.571	0.425	−0.056	−0.493	−0.569	−0.422	0.917	0.462	0.358	0.548
Peat-H	0.028	0.050	0.054	0.076	0.006	−0.025	−0.020	−0.072	0.974	0.893	0.854	0.825
PS23-H	0.038	0.356	0.332	0.319	−0.002	−0.331	−0.295	−0.286	0.993	0.893	0.854	0.825
PS14-H	0.090	0.271	0.192	0.227	−0.030	−0.268	−0.191	−0.226	0.959	0.673	0.783	0.741
Sand-H	0.228	0.488	0.590	0.457	−0.081	−0.453	−0.575	−0.411	0.825	0.484	0.364	0.544

RMSE: the root-mean square error, *AD*: the average deviations, and *NSE*: the Nash–Sutcliff Efficiency.
L and H suffixes low and high bulk densities.

comparison of measured and modeled λ(θ) for four soil types, including our new model and GD model simulations via estimated parameters based on two calculated methods above-mentioned. It seems the λ_{dry} play more significant role on determining the λ(θ) trend in our model than the GD model. Our model showed the gradual increase λ(θ) trend, but the convex curve became more dominant for the GD model. In contrast, while our model worked better than the GD model for the peat soil, the GD model performed better for the sandy soil. Interestingly, the geometric mean equation to estimate the λ_{dry} in our model performed much better than the λ_{dry} via the suggested empirical equations used in GD model, this confirmed the usefulness of geometric mean equation as the λ_{dry} is hard to predict. Nevertheless, further study of λ_{dry} is needed across several types of soil.

3.4. Model estimations

The accurate prediction of λ for different soil types, using our new model with the estimated parameters, required knowledge of only the lower and upper limits of λ (i.e., λ_{sat} and λ_{dry}). As such, the accurate estimation of λ_{sat} and λ_{dry} is crucial in our new model. The method of calculating λ_{sat} using the geometric mean equation has been well accepted, and using our model λ_{dry} can be predicted with the same level of accuracy as λ_{sat}, which confirms that the geometric mean equation can also be applied to estimate the λ_{dry}. In this way, the effect of organic/mineral content has been considered in analytical prediction methods using the contrasting thermal conductivity values of soil components (liquid, air, mineral and organic constituents) via a geometric mean equation.

Typically, the prediction of λ_{dry} is less accurate than that of λ_{sat}, due to qualifying complications which arise in variably porous media in a dry condition, as well as the lower weighting of air which mostly presents in the dry range in comparison to water which mostly presents in the wet range. While the calculation of λ_{sat} is similar in most models, the methods for determining λ_{dry} are very diverse. Fig. 5 shows a further comparison that was made between our proposed calculation of λ_{dry} and several other functions developed in previous studies, such as those of Johansen (1977); Cote and Konrad (2005), and Lu et al. (2007). Our proposed method actually performed better than other empirical models, which overestimate λ_{dry} for peat soil and underestimate λ_{dry} for sandy soil. Woodside and Messmer (1961) also found that the de Vries and the weighted geometric mean models predicted the porosity dependence of the λ_{dry} more accurately than other models. Usually, the Cote and Konrad (2005) and Lu et al. (2007) models could improve estimation of λ more effectively than Johansen (1977) model at lower water content, which also was not found in our study.

We also separately validated our new model by comparing the four models using the two peat:mineral mixes which were not used for our model derivation and calibration (Fig. 6). As expected, the new model with fitted parameters performed better than the other models, because the model parameters were derived from measured data. It is evident that the predicted λ values of the proposed model (i.e., the new model with estimated parameters) agree well with the λ measurements for both soil types. Table 3 shows that, for the PS41 soil treatment, the *NSE* of the proposed model is 0.576, which is similar to that of the de Vries model (0.523) and of the Cote and Konrad (2005) model (0.592). The proposed model gives better results than the other two models for the PS32 soil treatment, where the *NSE* of the proposed model is 0.4, which is higher than the *NSE* of the de Vries model (0.336) and the *NSE* of the Cote and Konrad (2005) model (0.337). Similar to the calibration result, our new model underestimated the measured value, which could be due to the underestimation of parameter values. Therefore, we conclude that although the values of λ_{dry} and λ_{sat} have a considerable effect on the development of the proposed model, our model is able to provide acceptable predictions of λ.

3.5. Model implications

Among the λ models discussed, it is clear that our new model is very applicable. Although the new model with the estimated parameters predicts similar results to the two other models, it is easier to use due to its simplicity. This implies that, to predict the λ, all models fit more-or-less equally well, providing their respective parameter values are optimized to specific soil data. In general, our new model offers several benefits over existing models:

1. The new model does not require any additional parameters, given that the two input parameters, i.e., the lower and upper limits of λ (λ_{dry} and λ_{sat}), are known or easily accessible. This is a very attractive and powerful feature. In contrast, the Cote and Konrad (2005) model requires the K_e value which are not always easy to obtain. Similarly, the de Vries (1963) model is complicated by the fact that each mineral constituent has unique values of λ and g.

2. The new model is mathematically continuous, in contrast to many other models that may not converge to λ_{dry} or λ_{sat}. In this case, our new model also provides values of thermal conductivity that respect the measured boundary limits of thermal conductivity for most soils.

3. The new model is physically-based given that the two parameters have strong physical meaning, i.e., boundary values of real soils. Our model is preferable to the Cote and Konrad (2005) model considering the two parameters are strongly associated with basic soil physical properties. When the complete peat/mineral composition is known, the λ of solid particles can be assessed by using the generalized geometric mean method with data for the thermal conductivity of forming materials.

4. The new model with fitted parameters performs best to predict the λ(θ) relationship for all sand and peat materials, followed by the Cote and Konrad (2005) model and the de Vries model; whereas the

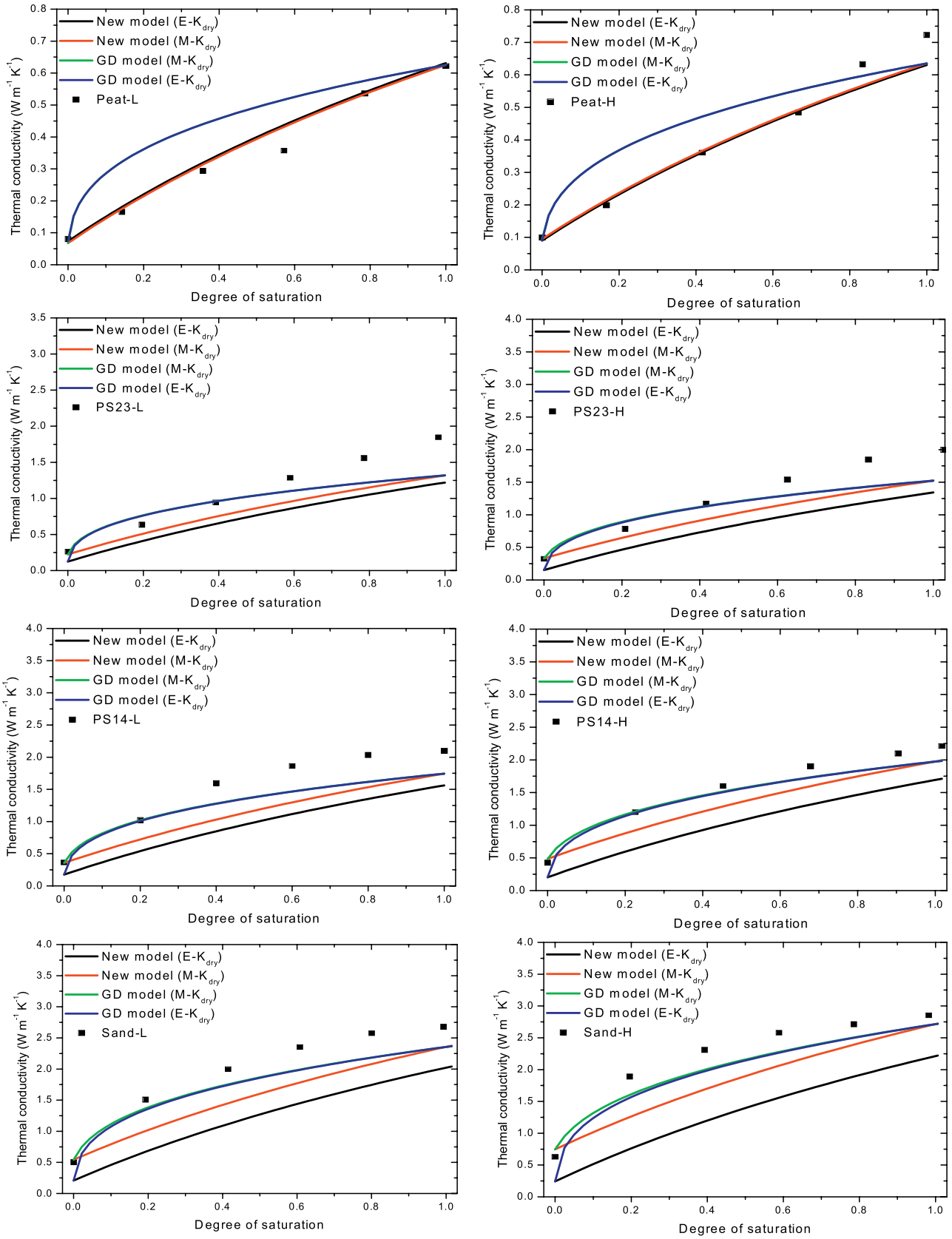

Fig. 4. A comparison of measured and modeled soil thermal conductivity-water content, (θ) relationships for four soil types, including the new model (estimated parameters), and Ghanbarian and Daigle (2016) model for four soil types. E-K_{dry} indicates the geometric mean equation applied to estimate the λ_{dry}, and M-K_{dry} indicates the empirical equations from Cote and Konrad (2005) applied to estimate the λ_{dry}. L and H indicate low and high bulk densities.

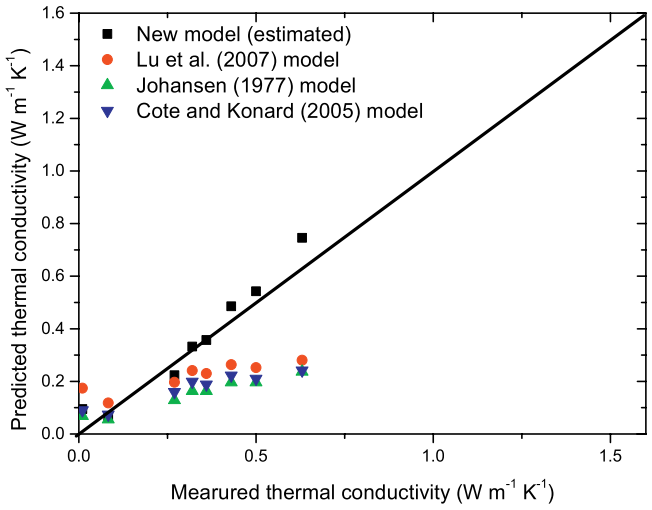
New model (estimated)
Lu et al. (2007) model
Johansen (1977) model
Cote and Konard (2005) model
Predicted thermal conductivity (W m-1 K-1)
Mearured thermal conductivity (W m-1 K-1)

Fig. 5. Comparison of measured and modelled soil dry thermal conductivity using the new model (estimated parameters), Lu et al. (2007) model, Johansen (1977) model, and Cote and Konrad (2005) model under four soil types (Peat, Sand, PS23 and PS14 at two different bulk densities).

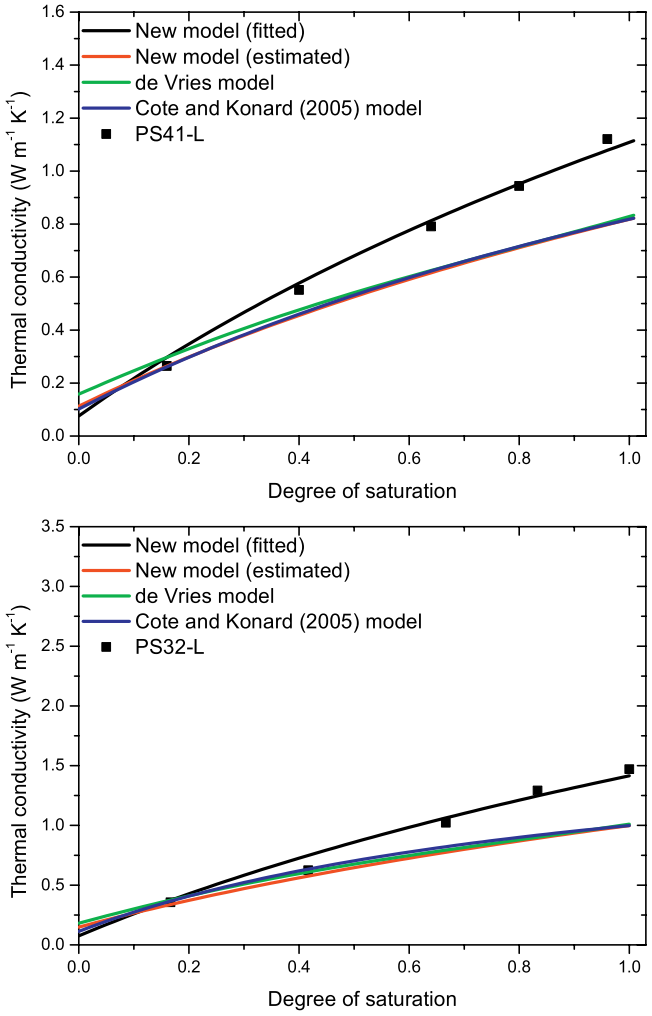

Fig. 6. A comparison of measured and predicted soil thermal conductivity-water content relationships for two soil types, including the new model (fitted and estimated parameters), de Vries model, and Cote and Konrad (2005) model. L indicates low bulk density.

new model with estimated parameters showed a similar level of accuracy among the three models, with a relatively high level of accuracy for dense sand.

The form of the primary equation in our model is theoretically applicable to either organic or mineral soils, under frozen or unfrozen conditions. Although the new model was derived based only on data from unfrozen soil measurements, the calculation processes within the model are also applicable to frozen soils. Further evaluation of the model's efficiency in frozen soils will be the focus of a future study. Due to the generalized form of the model and minimal number of input parameters, this method may be easily automated for the estimation of the λ used in numerical analyses of heat transfer in peatland in the cold area, and beyond.

The widely used models for estimating thermal conductivity require several input parameters, each associated with a marked measurement uncertainty, cost, and time. Notwithstanding, there is an increasing need for accurate and realistic heat transport models that require a minimum number of input parameters. Granberg et al. (1999) suggested that a better understanding of soil thermal properties is required if peat soil temperatures are to be more accurately estimated. The accurate simulation of temperatures is particularly important in the upper peat layers. This information is among the most crucial when making recommendations to the reclamation industries, relating to the design of appropriate soil covers which utilize peat:mineral mixes, and also important for the evaluation of carbon uptake and release in peat soils in the high latitude area (e.g., peat decomposition and methane production) (Kettridge and Baird, 2007). Our new model provides a beneficial contribution in that it addresses all of the above-stated issues. In addition, our research clearly demonstrates the necessity to further evaluate the physically-based λ(θ) relationships for a wider range of soil types. Although the current model accounted various soil compositions effects on the thermal conductivity, it is relatively limited in the qualification of soil mineralogy, which was found to be critically important (Bristow, 1998). For the sandy soil, all of the estimated values were greater than the measured ones, which may be reflecting that the measured values are not entirely representative of the true values (e.g., vapor movements). This situation raises an important uncertainty question as to whether the measured values are always preferred to the estimated values that are determined using a model, and should be investigated in future.

4. Conclusion

In this study we developed a simple but effective model for predicting soil thermal conductivity from knowledge of the soil moisture and other easily accessible properties such as sand content and dry bulk density. We proposed a functional relationship between the saturated (λ_{sat}) and non-saturated (λ_{dry}) thermal conductivities based on mineral/organic content, water content, and dry bulk density or other specific intrinsic soil properties, which can be easily provided using simple granulometric and gravimetric studies. If those bound limiting values are available for the investigated soil, then the new model may provide thermal estimations based solely on soil moisture, which may be significantly beneficial to hydrologic and climate models that utilize thermal property estimations.

The data from soils of known, controlled composition were analyzed in this study to test and validate a proposed λ model for permafrost sandy and peat soils in the high latitude area. The new model is capable of closely describing λ across the entire water content range for soils of various textures, where the *RMSE*s of the λ estimates are lower than those of the other commonly-used models that were tested in this study. For dense sandy soil, the new model showed a relatively high level of accuracy compared to the other models. Despite the simplicity of the model, its predictions are in good agreement with experimental results, and provide many advantages over other two tested models. Therefore, we conclude that the new model is not only capable of providing

Table 3
Model performance of evaluated samples based on *RMSE*, *AD* and *NSE* with the new model (fitted and estimated parameters), de Vries model, and Cote and Konrad (2005) model for four soil types. PS41 and PS32: ratio between peat and sand is 4:1 and 3:2, respectively.

Soil type	*RMSE*				*AD*				*NSE*			
(code)	Fitted	Esti -mated	de Vries	Cote and Konrad	Fitted	Esti -mated	de Vries	Cote and Konrad	Fitted	Esti -mated	de Vries	Cote and Konrad
PS41	0.028	0.199	0.193	0.196	0.009	−0.166	−0.151	−0.163	0.990	0.576	0.523	0.592
PS32	0.067	0.299	0.289	0.284	0.016	−0.237	−0.215	−0.206	0.967	0.400	0.336	0.337

RMSE: the root-mean square error, *AD*: the average deviations, and *NSE*: the Nash–Sutcliff Efficiency.

accurate estimates of λ for soils of various textures, but is more convenient and widely applicable than previous equations of λ in studying numerical algorithms for describing coupled heat and mass transfer processes. It can also be incorporated into global land surface models.

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